Monte Carlo Simulation for the EIC: Status and Experimental Requirements



Markus Diefenthaler





Measurements and simulations in experimental Nuclear Physics

Measurement



Simulation





Role of simulations in experimental Nuclear Physics



Design Experiments Design and develop detectors and large-scale detector systems based on key measurements / physics reach and background estimates. Optimize the design.

Analysis Develop and verify analysis methods and tools: Does the analysis tool or method give the corrector result? Estimate systematic uncertainties.

Verify Measurements Detailed simulations essential for commissioning experiments and verify analyses.

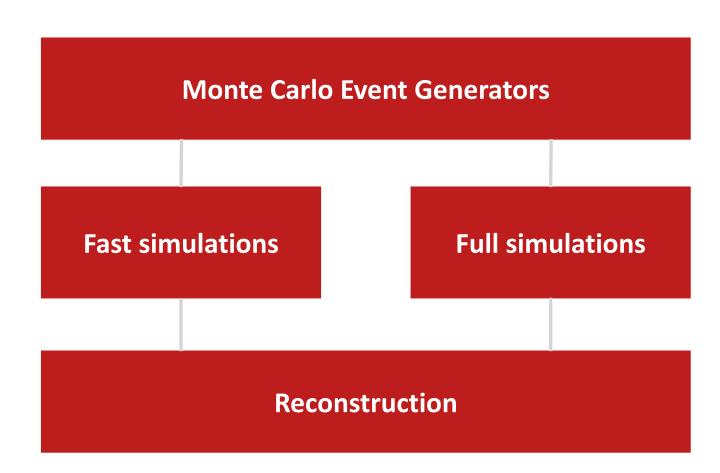


Simulation Software for the EIC

Simulation of physics processes

Simulation of detector responses

Analysis of simulated data

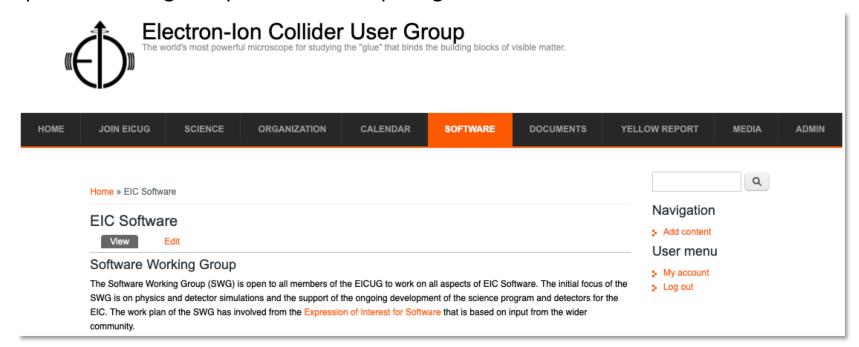




EIC R&D For Software & Computing

EIC Software & Computing is in a very early life stage:

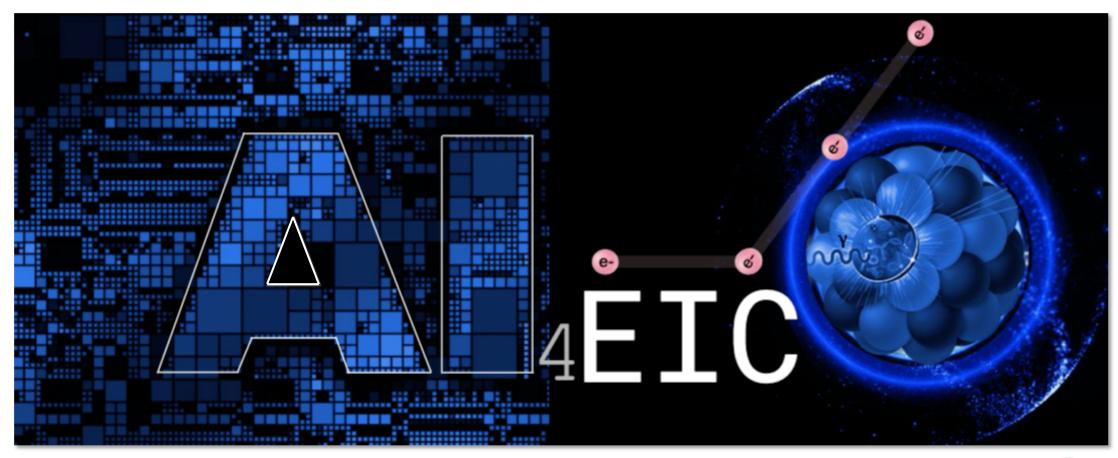
- The current focus is supporting detector design.
- <u>Software Working Group</u> (SWG) within the EIC User Group works with the community and proto-collaborations to address software needs and evolving R&D.
- Legacy codes and frameworks are in use.
- Distributed Computing approach to supply resources for physics detector studies.
- At the pre-requirements stage for production computing and software activities.





AI/ML for EIC

AI/ML already has an important presence in EIC, with one of the proto-collaborations (ECCE) applying it to detector design optimization, as well as applications such as streaming DAQ, and a **new** AI Working Group as part of SWG to explore and develop AI/ML's potential.



Driven by community need, 'bottom up'



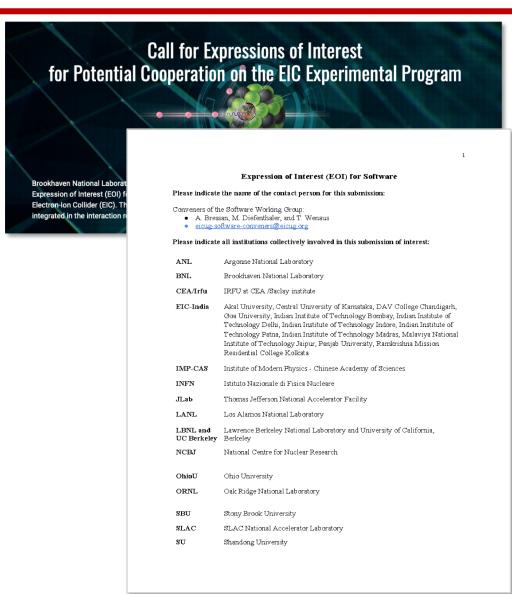
The Software Working Group collected information on the community's specific software tools and practices during the Yellow Report Initiative.

Q7. Do you have any <u>comments</u> on your current experience with EIC Software?

Common message:
Priorities for consolidating around common software are in MC generators and detector simulation



EIC Common Software: The Software EOI (and 'living' planning document)



- Software Tools for Simulations and Reconstruction
 - Monte Carlo Event Generators
 - Detector Simulations
 - Reconstruction
 - Validation
- Middleware and Preservation
 - Workflows
 - Data and Analysis Preservation
- Interaction with the Software Tools
 - Explore User-Centered Design
 - Discoverable Software cvmfs/spack
 - Data Model
- Future Technologies
 - Heterogeneous computing
 - New languages and tools
 - Collaborative software

https://indico.bnl.gov/event/8552/contributions/43221/



MCEG Distribution for the EIC



EIC community has been organized around its MCEGs needs already for several years:

- PYTHIA6 (modified)
- BeAGLE
- DJANGOH
- elSpectro
- eSTARlight
- MILOU
- PEPSI
- RAPGAP
- Sartre
- TOPEG (Orsay Perugia)

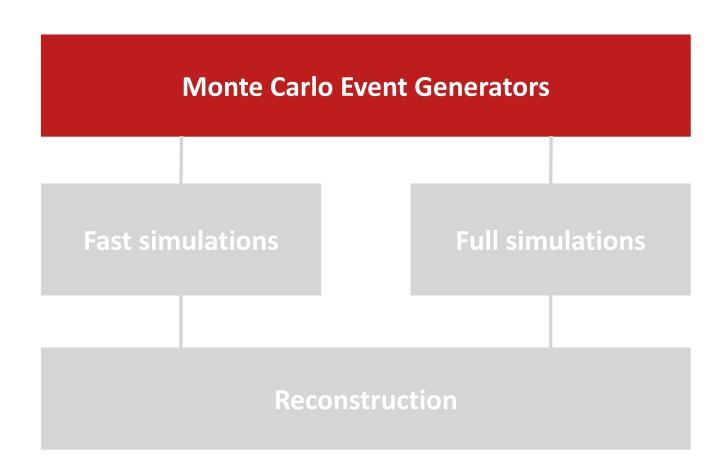
Maintained on CVMFS and used for a plethora of EIC studies. Established HepMC2/3 as standard in the wider EIC community (thanks to Andrii Verbytskyi (MPP) for support).

Discussion of Event Generation and Simulation Needs

Simulation of physics processes

Simulation of detector responses

Analysis of simulated data





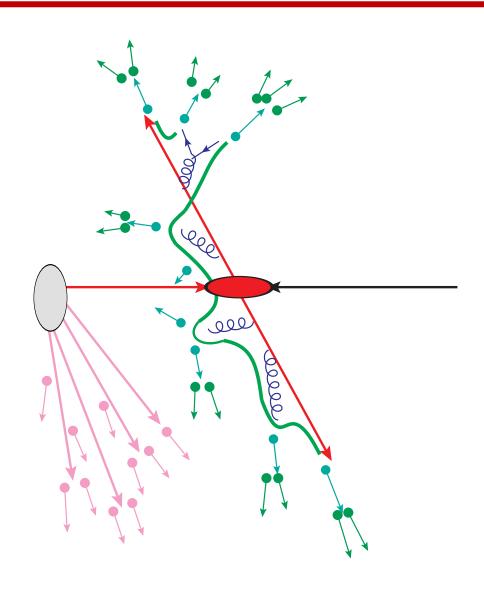
Monte Carlo Event Generator

MCEG

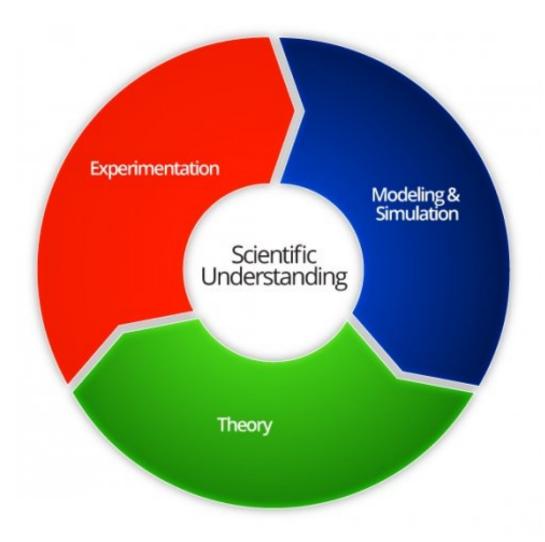
- faithful representation of QCD dynamics
- based on QCD factorization and evolution equations

MCEG algorithm

- 1. Generate kinematics according to fixed-order matrix elements and a PDF. Session on "The Role of PDFs"
- 2. QCD Evolution via parton shower model (resummation of soft gluons and parton-parton scatterings). Session on "The Role of Parton Showers"
- 3. Hadronize all outgoing partons including the remnants according to a model. Session on "The Role of Hadronization"
- 4. Decay unstable hadrons.



Event Generators for the EIC



Monte Carlo Simulation of

- electron-proton (ep) collisions,
- electron-ion (eA) collisions, both light and heavy ions,
- including higher order QED and QCD effects,
- including a plethora of spin-dependent effects.

Common challenges, e.g. with HL-LHC: High-precision QCD measurements require high-precision simulations.

Unique challenges MCEGs for electron-ion collisions and **spin-dependent** measurements, including novel QCD phenomena (e.g., GPDs or TMDs).



Start building a MCEG community for the EIC



Satellite workshop during POETIC 8





Organized by Elke-Caroline Aschenauer (BNL), Andrea Bressan (Trieste), Markus Diefenthaler (JLab), Hannes Jung (DESY), Simon Plätzer (Vienna), Stefan Prestel (LUND)

Summary from MCEG workshop series

MCEG for ep On a good path, but still a lot of work ahead.

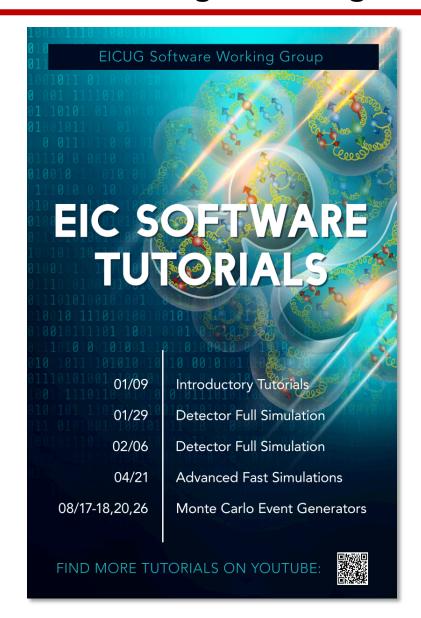
- General-purpose MCEGs, HERWIG, PYTHIA, and SHERPA, will be significantly improved w.r.t. MCEGs at HERA time:
- Comparisons with HERA data and QCD predictions critical:
 - To learn where physics models need to be improved,
 - To complement MC standard tunes with first DIS/HERA tune.
- The existing general-purpose MCEG should be able to simulate NC and CC unpolarized observables also for eA. A precise treatment of the nucleus and, e.g., its breakup is needed.
- First parton showers and hadronization models for ep with spin effects, but far more work needed for polarized ep / eA simulations.
- Need to clarify the details about merging higher QED+QCD effects (in particular for eA).

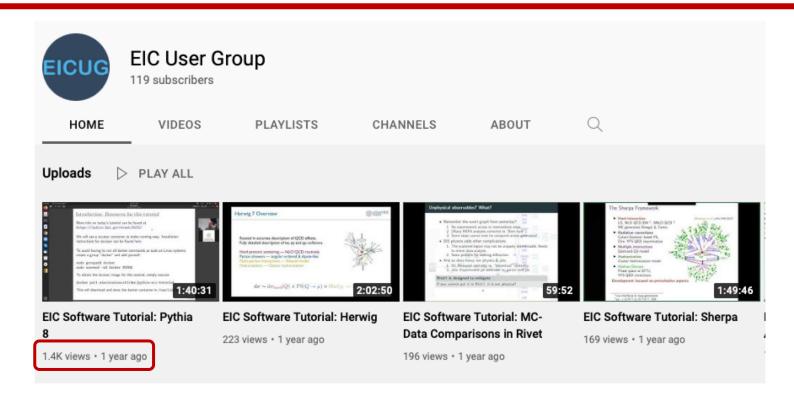
MCEG for eA Less clear situation about theory and MCEG.

- Pioneering projects, e.g., BeAGLE, spectator tagging in ed, Sartre.
- Active development, e.g., eA adaptation of JETSCAPE, Mueller dipole formalism in Pythia8 (ala DIPSY).



Introducing modern general-purpose MCEGs and Rivet



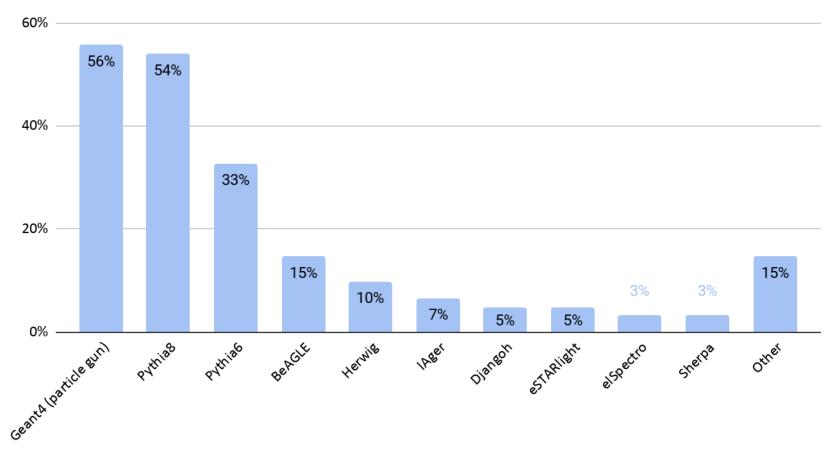


Excellent feedback on online tutorials and their recordings.

MCEGs used for Yellow Report

Source State of Software Survey





Other (N = 9): personal computer codes (N = 2), ACT, CLASDIS, ComptonRad, GRAPE-DILEPTON, MADX, MILOU, OPERA, RAYTRACE, Sartre, Topeg, ZGOUBI

MCEG R&D requires easy access to data:

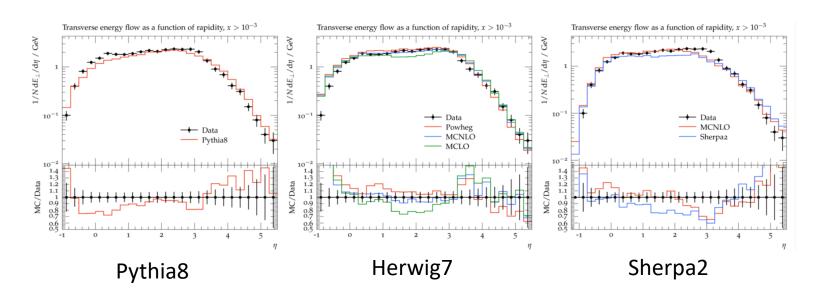
→ Rivet talk by Andy Buckley

• data := analysis description + data points

HEP existing workflow using Rivet.

Ongoing activity with EIC-India and MCnet:

- Comparison to published results using RIVET and understand differences.
- Provide initial findings and results in publication (work in progress)::
 - Overview of where we stand in understanding HERA data with current physics and models implement in MCEGs.

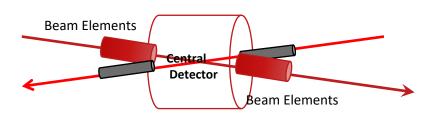




Machine-Detector interface (MDI)

Integrated interaction region and detector design to optimize physics reach

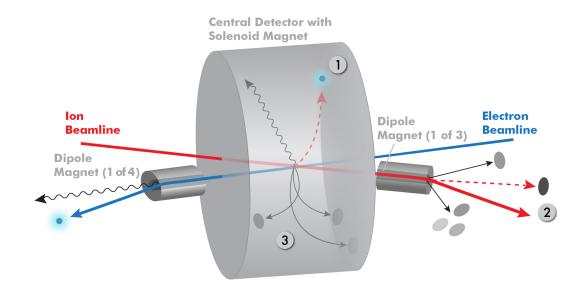
The aim is to get ~100% acceptance for all final state particles, and measure them with good resolution.



Experimental challenges:

- beam elements limit forward acceptance
- central Solenoid not effective for forward

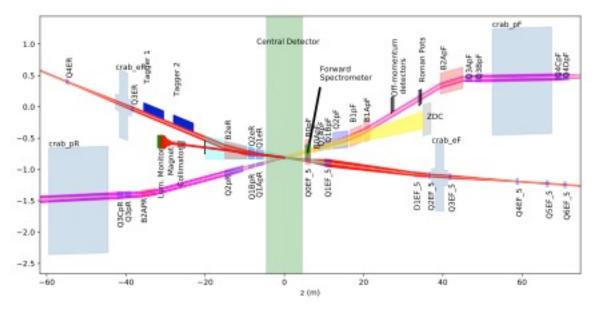
Possible to get ~100% acceptance for the whole event.





MDI in Simulations

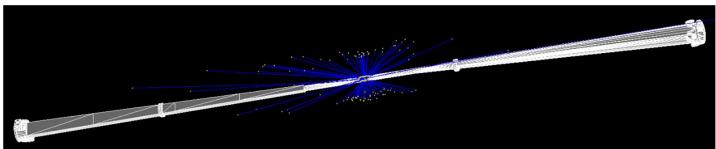
IR Layout

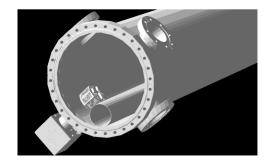


Unprecedented integration of IR and detector (shown here for IP6).

CAD Interface

(accelerator elements and service structures)



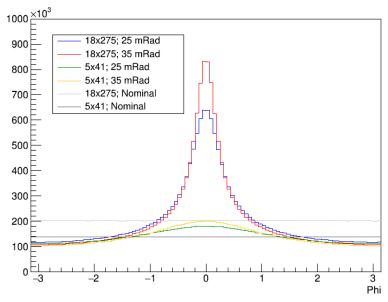


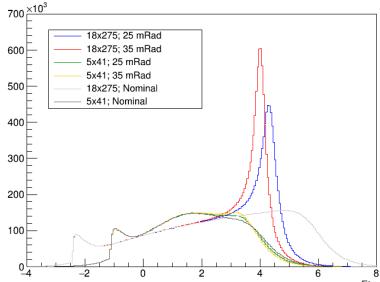
EIC Project

Simulation based (in part) on CAD files provided by EIC project engineering teams, rather than a bottoms-up reliance on constructive solid geometry (Screenshots from **eAST**)



Accelerator and Beam Conditions Critical for EIC Simulations





- Accelerator and beam effects that influence EIC measurements
 - Beam crossing angle,
 - Crabbing rotation,
 - Beam energy spread,
 - Angular beam divergence,
 - Beam vertex spread.
- Note for EIC Community https://eic.github.io/resources/simulations.html
 - Profound consequences on measurement capabilities of the EIC and layout of the detectors,
 - How to integrate these effects in EIC simulations.
 - **Authors** J. Adam, E.-C.Aschenauer, M. Diefenthaler, Y. Furletova, J. Huang, A. Jentsch, B. Page.

Beyond that Include beam background estimates in simulations.

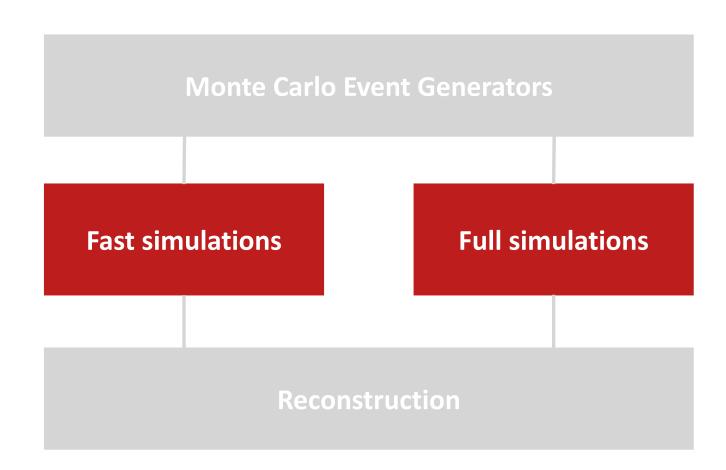


Discussion of Event Generation and Simulation Needs

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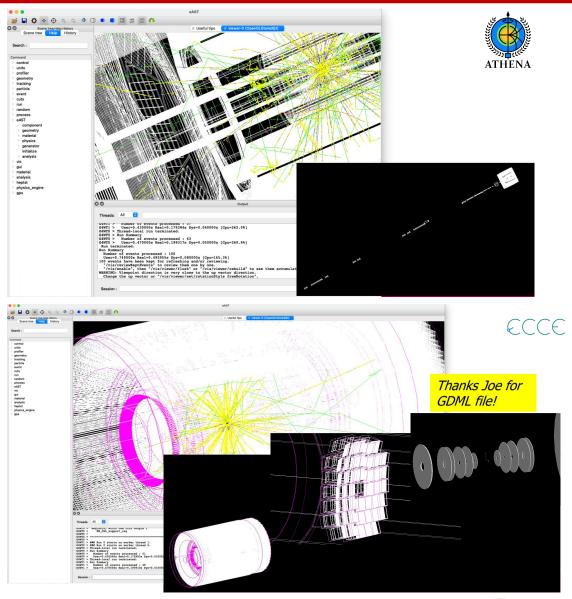




Detector simulations and Geant4

EIC

- Detector (and physics) simulations rely on Geant4,
 the (!) detector simulation toolkit for HEP and NP:
 - Detector full simulations for ATHENA and ECCE detector concepts based on Geant4.
 - As GeantV comes up at times:
 - Project <u>concluded</u>: no performance gain from the vectorization of the individual software components,
 - Modular software packages such as VecGeom integrated into Geant4.
- Energy range is different from LHC,
- validation, tuning and extension including test beam studies required.
- Ongoing collaboration with international Geant4 collaboration, including Technical Forum on NP/EIC.



Towards a Next-Generation Simulations



There are too many generators and simulation tools used at the moment.

Unify the Simulation Effort

- The SWG is preparing to launch a **common effort on next-generation simulations**:
 - building on the work done in the existing simulations,
 - unify the software community behind one common effort,
 - a requirement for the common framework is that it integrate the existing detector simulations in a modular way.





Project eAST in a nutshell

20 developers and growing

Detector Simulation

- comprehensive, centrally maintained application
- based on Geant4 for fast and full simulations
- with library of potential detector options

Requirements

- ability to reuse existing simulation work
- ease of switching detector options
- ease of switching between detailed and coarse detector descriptions
- ease of leveraging new and rapidly evolving technologies,
 - AI/ML to accelerate simulations
 - computing hardware, e.g., heterogeneous architectures
 - AI/ML is the best near term prospect for using LCF/Exascale effectively

Project Leader

 Makoto Asai, Geant4 project leader and deep technical expert for >20yrs.



The role of AI/ML in simulations

Lesson learned High-precision QCD measurements require high-precision simulations

Statistical accuracy for precise hypothesis testing

- up to trillion of simulated events required (HL-LHC)
- often computationally intensive, in particular calorimeter simulations

Common alternatives

- fast simulations with computationally efficient approximations, e.g., parameterizations or look-up tables
- still insufficient accuracy for high-precision measurements

Promising alternatives

- fast generative models, e.g., GANs or VAEs
- Al driven design, e.g., Bayesian optimization

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Review

A.I. for nuclear physics

Paulo Bedaque¹, Amber Boehnlein^{2,a}@, Mario Cromaz³, Markus Diefenthaler², Latifa Elouadrhiri², Tanja Horn⁴, Michelle Kuchera⁵, David Lawrence⁵, Poen Leé⁶, Steven Lidia⁶, Robert McKeown², Wally Melnitchouk², Witold Nazarewicz⁶, Kostas Orginos^{2,7}, Vyes Roblin⁷, Michael Scott Smith⁸, Malachi Schram⁹, Xin-Nian Wang³

- 1 University of Maryland, College Park, MD, USA
- ² Thomas Jefferson National Accelerator Facility, Newport News, VA, USA
- ³ Lawrence Berkeley National Laboratory, Berkeley, CA, USA
- ⁴ Catholic University, Washington D.C., USA
- 5 Davidson College, Davidson, NC, USA
- Michigan State University, East Lansing, MI, USA
- Ollege of William & Mary, Williamsburg, VA, USA Oak Ridge National Laboratory, Oak Ridge, TN, USA
- 9 Pacific Northwest National Laboratory, Richland, WA, USA

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Abstract This report is an outcome of the workshop AI for Nuclear Physics held at Thomas Jefferson National Accelerator Facility on March 4–6. 2020

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This report is an outcome of the workshop AI for Nuclear Physics held at Thomas Jefferson National Accelerator Facility on March 4–6, 2020. The workshop brought together 184 scientists to explore opportunities for Nuclear Physics in the area of Artificial Intelligence. The workshop consisted of plenary talks, as well as six working groups.

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a e-mail: amber@jlab.org (corresponding author)

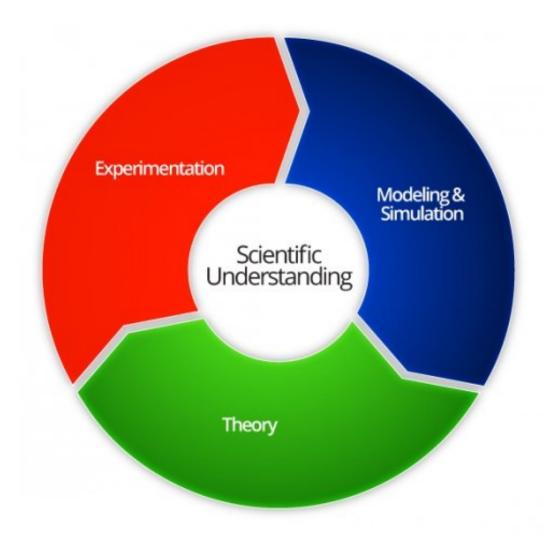
Bringing experts in various domains of QCD theory and experiment together

"It will be joint progress of theory and experiment that moves us forward, not in one side alone" Donald Geesaman (ANL, former NSAC Chair) on "Nuclear Physics in a Decade"

Open Questions

- How will we compare theory and experiment at the EIC?
 - Will we unfold our experimental measurements to Born level and compare them to theoretical calculations at Born level? This has been done at HERA.
 - Will we fold the theoretical calculations with radiative and detector effects and compare them at detector level? This has been done for NP and being developed further, e.g., [arXiv:2108.13371]. This is also being discussed for LHC.
 - This has profound consequences on the reproducibility and reinterpretability of our measurements and the requirements on our analysis software and workflows.
- How will we evaluate PDFs and FFs at the EIC?
 - Can we have a "LHAPDF" type of interface for PDF and FFs, including nuclear, spin-dependent, transverse-momentum dependent effects? We need this for LO, NLO, and beyond.
 - Can we use ML to parametrize all of this information, including uncertainties, in a computationally efficient way?
- Do we understand the limitations of measurements at the EIC?
 - We are better and better understanding the measurement capabilities of the EIC detectors.
 - What about the theoretical limitations of the measurements? How can we address them?

Towards high-precision simulations for the EIC





Next steps for MC4EIC

- Discuss requirements for MCEGs and related computations tools to simulate the collision of highly-polarized electrons and highly-polarized light ions and unpolarized heavy ions.
- Develop a roadmap for MCEG developments for the EIC, including HEP-NP funding.
- Priorities for the next years could be:
 - Training of the EIC community, e.g., via online tutorials.
 - Validation of existing MCEGs using Rivet. Build automated workflows (CI/CD).
 - Development of a DIS tune.
 - Merging of higher order QED and QCD effects.
 - Interface between MCEGs and Geant4 based on HepMC3.
 - Roadmap for spin-dependent parton showers.
 - Roadmap for spin-dependent hadronization models.
 - Guidance on how to compare measurements at the EIC with theory.



Summary

mdiefent@jlab.org



- **Simulations** essential for design of experiments, data analysis, and verification of measurements.
- **Simulations** for the **EIC**, i.e. MCEGs and fast and full detector simulations for the EIC, require **R&D**. We miss core capabilities and we need to work towards accuracy and precision.
- Simulation R&D is most efficiently done in common projects and in collaboration with other fields, in particular HEP.
- Many opportunities for AI/ML to complement and improve **simulations**. While AI/ML approaches will substitute parts of our **simulation workflows**, they will not replace core tools, e.g., general-purpose MCEGs or Geant4.







